An analysis of the Grünwald–Letnikov scheme for initial-value problems with weakly singular solutions

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Abstract

A convergence analysis is given for the Grünwald-Letnikov discretisation of a Riemann-Liouville fractional initial-value problem on a uniform mesh $t_m = m\tau$ with $m = 0, 1, \ldots, M$. For given smooth data, the unknown solution of the problem will usually have a weak singularity at the initial time $t = 0$. Our analysis is the first to prove a convergence result for this method while assuming such non-smooth behaviour in the unknown solution. In part our study imitates previous analyses of the L1 discretisation of such problems, but the introduction of some additional ideas enables exact formulas for the stability multipliers in the Grünwald-Letnikov analysis to be obtained (the earlier L1 analyses yielded only estimates of their stability multipliers). Armed with this information, it is shown that the solution computed by the Grünwald-Letnikov scheme is $O(\tau t_m^{\alpha-1})$ at each mesh point t_m; hence the scheme is globally only $O(\tau^\alpha)$ accurate, but it is $O(\tau)$ accurate for mesh points t_m that are bounded away from $t = 0$. Numerical results for a test example show that these theoretical results are sharp.

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1. Introduction

There is great current interest in the numerical solution of differential equations that involve fractional-order derivatives. One type of fractional derivative that has received much attention is the Riemann-Liouville derivative. An old and well-known discretisation of this derivative is the Grünwald-Letnikov (GL) formula [1, Section 2.4], which has been

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mentioned frequently in the research literature, yet there has been no rigorous analysis of the accuracy of this discretisation when it is applied to a Riemann-Liouville fractional initial-value problem with a solution that is typical for given smooth data — that is, a solution that exhibits a weak singularity at the initial time $t = 0$ (see Remark 3.2).

The *truncation error* of the GL scheme for certain smooth functions is examined in [2, 3], and for the function t^σ (for an arbitrary constant $\sigma \geq 0$) in [4, Lemma 2.1], but these investigations still leave unanswered the question of what *convergence rate* is attained by the scheme when applied to a problem with a weakly singular solution.

We shall consider the Grünwald-Letnikov discretisation of a Riemann-Liouville fractional initial-value problem on a uniform mesh, for given smooth data. Our analysis uses some ideas from [5, 6], which analyse the well-known L1 scheme. But in the case of the GL scheme, we have the remarkable new result that the stability multipliers in the analysis can be determined *exactly;* in [6] and related analyses such as [7], one can prove only upper bounds for these multipliers.

The paper is structured as follows. The Grünwald-Letnikov scheme (on a uniform mesh of diameter τ) and some of its properties are described in Section 2. In Section 3 we formulate the initial-value problem and derive a decomposition of its solution. Then a simple analysis of the Grünwald-Letnikov scheme shows that its computed solution is at least $O(\tau^\alpha)$ accurate at each mesh point. Next, in Section 4, we perform a more sophisticated analysis of the scheme which involves stability multipliers; a novel argument using generating functions enables us to calculate exactly the stability multipliers for the scheme, and we use this valuable information to show that the computed solution is $O(\tau t_m^{\alpha-1})$ at each mesh point t_m. Consequently the scheme is $O(\tau)$ accurate for mesh points t_m that are bounded away from $t = 0$. Finally, a numerical test problem in Section 5 shows that our theoretical results are sharp.

Notation. Set $\mathbb{N} := \{1, 2, \dots\}$ and $\mathbb{N}_0 := \{0, 1, 2, \dots\}$. For each $r \in \mathbb{R}$, we denote by $\lceil r \rceil$ the smallest integer satisfying $r \leq \lceil r \rceil$. We use C to denote a generic positive constant that can take different values in different places, but is always independent of the mesh. By $f_m \lesssim g_m$ we mean $f_m \leq C g_m$ for all m and some fixed positive constant C.

2. The Grünwald-Letnikov scheme

Let $\alpha > 0$ be fixed. For suitable functions v defined on the interval $[0, T]$, the Grünwald-Letnikov (GL) fractional derivative of order α of v at each point $t > 0$ is defined [1, Definition 2.3] by

$$D^\alpha_{GL} v(t) = \lim_{M \to \infty} \frac{1}{\tau_M^\alpha} \sum_{k=0}^{M} (-1)^k \binom{\alpha}{k} v(t - k\tau_M), \tag{2.1}$$

where $\tau_M = t/M$.

The Riemann-Liouville integral operator I^β is defined for each $\beta > 0$ by

$$I^\beta w(t) := \frac{1}{\Gamma(\beta)} \int_0^t (t-s)^{\beta-1} w(s) \, \mathrm{d}s.$$

If $v \in C^{\lceil \alpha \rceil}[0,T]$, then by [1, Theorem 2.25] one has $D^\alpha_{GL} v(t) = D^\alpha_{RL} v(t)$, the Riemann-Liouville derivative of v, which is defined by $D^\alpha_{RL} w(t) := \frac{d}{dt}\left(I^{1-\alpha} w\right)(t)$.

The GL finite difference operator L^α_t is obtained by taking a finite value of M in (2.1), as we now describe. Let M be a positive integer. Set $\tau = T/M$ and $t_m = m\tau$ for $m = 0, 1, \ldots, M$, so the mesh $\{t_m : m = 0, 1, \ldots, M\}$ is uniform. Then for any mesh function $\{V_j\}_{j=0}^M$, set

$$L^\alpha_t V_m := \frac{1}{\tau^\alpha} \sum_{k=0}^{m} \omega_k^{(\alpha)} V_{m-k} \quad \text{for } m = 1, \ldots M, \quad \text{where } \omega_k^{(\alpha)} := (-1)^k \binom{\alpha}{k}. \tag{2.2}$$

Thus for a given function v defined on $[0,T]$, the GL finite difference approximation of $D^\alpha_{RL} v(t_m)$ is $L^\alpha_t v(t_m)$.

Assumption 2.1. *We take $0 < \alpha < 1$ in the rest of the paper.*

For our later analysis, we first derive a useful property of the coefficients $\omega_k^{(\alpha)}$ in (2.2). Set

$$d_k^{(\alpha)} = \frac{\Gamma(k-\alpha)}{\Gamma(1-\alpha)\Gamma(k)} \quad \text{for } k = 1, 2, \ldots \tag{2.3}$$

Note that $d_1^{(\alpha)} = 1$. We also define $d_0^{(\alpha)} = 0$; this is consistent with the formula (2.3) as $\Gamma(0)$ is infinite. Gautschi's inequality [8] applied to (2.3) yields

$$\frac{k^{-\alpha}}{\Gamma(1-\alpha)} < d_k^{(\alpha)} < \frac{(k-1)^{-\alpha}}{\Gamma(1-\alpha)} \quad \text{for } k = 1, 2, \ldots \tag{2.4}$$

From this inequality (or from an inspection of $d_k^{(\alpha)}$) it is immediate that $d_k^{(\alpha)} > d_{k+1}^{(\alpha)}$ for $k = 1, 2, \ldots$.

Lemma 2.1. *One has $\omega_k^{(\alpha)} = d_{k+1}^{(\alpha)} - d_k^{(\alpha)}$ for $k = 1, 2, \ldots$*

Proof. Using the well-known property $x\Gamma(x) = \Gamma(x+1)$ for all $x \in \mathbb{R}$ with x not a nonpositive integer, we get

$$\begin{aligned}
d_{k+1}^{(\alpha)} - d_k^{(\alpha)} &= \frac{\Gamma(k+1-\alpha)}{\Gamma(1-\alpha)\Gamma(k+1)} - \frac{\Gamma(k-\alpha)}{\Gamma(1-\alpha)\Gamma(k)} = \frac{(k-\alpha)\Gamma(k-\alpha)}{-\alpha\Gamma(-\alpha)\Gamma(k+1)} - \frac{k\Gamma(k-\alpha)}{-\alpha\Gamma(-\alpha)\Gamma(k+1)} \\
&= \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)} \\
&= \omega_k^{(\alpha)}
\end{aligned}$$

from the definition of $\omega_k^{(\alpha)}$ in (2.2) — see, e.g., [3, eq. (6)]. □

Lemma 2.1 and $\omega_0^{(\alpha)} = 1$ enable us to rewrite the definition (2.2) of L^α_t as

$$L^\alpha_t V_m = \frac{1}{\tau^\alpha} \left[V_m - \sum_{k=1}^{m} (d_k^{(\alpha)} - d_{k+1}^{(\alpha)}) V_{m-k} \right] \quad \text{for } m = 1, \ldots M, \tag{2.5}$$

where we remind the reader that $d_k^{(\alpha)} - d_{k+1}^{(\alpha)} > 0$ for each k.

Our next result is a discrete stability inequality for the operator L^α_t. It imitates the analogous result for the well-known L1 discretization that is obtained in [5, Lemma 2.1].

Lemma 2.2. *For any mesh function* $\{V_j\}_{j=0}^M$ *with* $V_0 = 0$*, one has*

$$|V_k| \le \Gamma(1-\alpha) \max_{j=1,\dots,k} \{t_j^\alpha L_t^\alpha |V_j|\} \quad \text{for} \quad k = 1, \dots, M.$$

Proof. Fix $k \in \{1, 2, \dots, M\}$. Suppose $\max_{j=1,\dots,k} |V_j| = |V_n|$ for some $n \in \{1, \dots, k\}$. Since $V_0 = 0$, the formula (2.5) becomes

$$\begin{aligned} L_t^\alpha |V_n| &= \frac{1}{\tau^\alpha} \left[|V_n| - \sum_{k=1}^{n-1} (d_k^{(\alpha)} - d_{k+1}^{(\alpha)}) |V_{n-k}| \right] \\ &\ge \frac{1}{\tau^\alpha} \left[|V_n| - \sum_{k=1}^{n-1} (d_k^{(\alpha)} - d_{k+1}^{(\alpha)}) |V_n| \right] \\ &= \frac{1}{\tau^\alpha} d_n^{(\alpha)} |V_n|, \end{aligned}$$

where we used $d_k^{(\alpha)} - d_{k+1}^{(\alpha)} > 0$ and $|V_n| \ge |V_{n-k}|$. That is, $|V_n| \le \tau^\alpha (d_n^{(\alpha)})^{-1} L_t^\alpha |V_n|$. The result now follows from (2.4). $\square$

3. A fractional initial-value problem

Recall that $\alpha \in (0, 1)$. Consider the fractional initial-value problem

$$D_{RL}^\alpha u(t) + c(t) u(t) = f(t) \quad \text{for } 0 < t \le T, \tag{3.1a}$$

$$u(0) = 0, \tag{3.1b}$$

where $c \in C^2[0, T]$ and $f \in C^2[0, T]$ are given with $c \ge 0$ on $[0, T]$. In (3.1b) the choice of initial condition is not arbitrary: we desire to study solutions u of (3.1a) that lie in $C[0, T]$, which implies $D_{RL}^\alpha u \in C[0, T]$ since $c, f \in C[0, T]$, and consequently [9, Corollary 1] (which is a slight extension of [10, Section 4]) tells us that one must have $u(0) = 0$.

Remark 3.1. *The initial condition* $u(0) = 0$ *implies that* $D_{RL}^\alpha u(t) = D_C^\alpha u(t)$*, the Caputo derivative of* u *which is defined by* $D_C^\alpha u(t) := I^{1-\alpha} u'(t)$*; see [1, Lemma 3.5]. Thus* (3.1) *may be regarded as a Riemann-Liouville initial-value problem or as a Caputo initial-value problem.*

It is well known that (3.1) is equivalent to the weakly singular Volterra integral equation

$$u(t) = g(t) - I^\alpha (cu)(t) \quad \text{for } 0 \le t \le T, \tag{3.2}$$

where $g(t) := I^\alpha f(t)$. Write $f(t) = f(0) + t f'(0) + Q_2(t)$, where $Q_2(t) := \int_{s=0}^t f''(s)(t - s)\, \mathrm{d}s$. Then

$$\begin{aligned} (I^\alpha Q_2)(t) &= \frac{1}{\Gamma(\alpha)} \int_{r=0}^t (t-r)^{\alpha-1} \int_{s=0}^r f''(s)(r-s)\, \mathrm{d}s\, \mathrm{d}r \\ &= \frac{1}{\Gamma(\alpha)} \int_{s=0}^t f''(s) \int_{r=s}^t (t-r)^{\alpha-1} (r-s)\, \mathrm{d}r\, \mathrm{d}s \\ &= \frac{1}{\Gamma(2+\alpha)} \int_{s=0}^t f''(s)(t-s)^{\alpha+1}\, \mathrm{d}s, \end{aligned}$$

by a standard formula for the Beta function [1, Theorem D.6]. It is now clear that $I^\alpha Q_2 \in C^2[0,T]$. Hence

$$g(t) = k_0 t^\alpha + k_1 t^{1+\alpha} + \psi(t) \quad \text{for } t \in [0,T], \tag{3.3}$$

where k_0, k_1 are some constants and $\psi \in C^2[0,T]$. From [11, Theorem 6.1.2] the solution of (3.2) is

$$u(t) = g(t) + \int_{s=0}^{t} R_{1-\alpha}(t,s) g(s)\,\mathrm{d}s, \tag{3.4}$$

where $R_{1-\alpha}(t,s) = (t-s)^{\alpha-1}\sum_{n=1}^{\infty}(t-s)^{(n-1)\alpha}\Phi_n(t,s;1-\alpha)$, with $\Phi_n(\cdot,\cdot;1-\alpha) \in C^2\big([0,T]^2\big)$ for each n because $c \in C^2[0,T]$ (see [11, p.347]). Substituting (3.3) into (3.4) and imitating the proof of [11, Theorem 6.1.6(ii)], we obtain

$$u(t) = \sum_{(j,k)_\alpha} \gamma_{j,k} t^{j+k\alpha} + Y_2(t;\alpha) \quad \text{for } 0 \le t \le T, \tag{3.5}$$

where $(j,k)_\alpha := \{(j,k) : j,k \in \mathbb{N}_0, j + k\alpha < 2\}$, the coefficients $\gamma_{j,k}$ are some constants, and the function Y_2 has the properties that

$$Y_2(\cdot\,;\alpha) \in C^2[0,T] \quad \text{and} \quad 0 = Y_2(0;\alpha) = \left.\frac{dY_2(t;\alpha)}{dt}\right|_{t=0}. \tag{3.6}$$

Note that $u(0) = 0$ implies that $\gamma_{0,0} = 0$ in (3.5); we shall need this property in Lemma 3.2.

Remark 3.2. *The formula* (3.5) *shows that a typical solution u of* (3.1) *will include a term $\gamma_{0,1}t^\alpha$ in its decomposition. Thus u lies in $C[0,1]$, but not in $C^1[0,1]$ since $u'(t)$ will blow up as $t \to 0^+$.*

Remark 3.3. *Decompositions of solutions of related problems appear in [12, 13, 14]. Our analysis needs more fine detail than appears in these sources, so we base it on [11] where one finds the most explicit description of the terms appearing in the decomposition of the solution.*

To discretise (3.1) we use the GL scheme (2.2) on the uniform mesh $t_m = m\tau$ of Section 2, viz.,

$$L_t^\alpha U_m + c_m U_m = f_m \quad \text{for } m = 1, \dots M, \tag{3.7a}$$

$$U_0 = 0, \tag{3.7b}$$

where $c_m := c(t_m)$ and similarly for f. The solution of (3.7) is $U_0, U_1, \dots, U_M$. It is clear from (2.5) and $c \ge 0$ that for each $m \ge 1$, the value of U_m is determined uniquely by (3.7a) using the values $U_0, U_1, \dots, U_{m-1}$.

The truncation error of the GL approximation of the Riemann-Liouville derivative is described for certain functions in the following result.

Lemma 3.1. *[4, Lemma 2.1] Let* $v(t) = t^\sigma$ *where* $\sigma \geq 0$ *is a constant. Then*

$$D_{RL}^\alpha v(t_m) = L_t^\alpha v(t_m) + \tau \frac{\alpha\Gamma(\sigma+1)}{2\Gamma(\sigma-\alpha)} t_m^{\sigma-1-\alpha} + \tau^2 R^{m,\alpha,\sigma}, \tag{3.8}$$

where $|R^{m,\alpha,\sigma}| \leq C t_m^{\sigma-2-\alpha}$ *for some constant* C *that is independent of* m *and* τ.

This result enables us to give a truncation error bound for the non-smooth terms $\sum_{j,k} \gamma_{j,k} t^{j+k\alpha}$ in (3.5).

Lemma 3.2. *Set* $z(t) = \sum_{(j,k)_\alpha} \gamma_{j,k} t^{j+k\alpha}$ *for* $t \in [0,T]$, *where we recall that* $\gamma_{0,0} = 0$. *Set* $\gamma = \min\{1, 2\alpha\}$. *Then*

$$|D_{RL}^\alpha z(t_m) - L_t^\alpha z(t_m)| \lesssim m^{-2} + \tau^{\gamma-\alpha} m^{-(1+\alpha-\gamma)} \quad \textit{for } m = 1, 2, \ldots, M.$$

Proof. Since $\gamma_{0,0} = 0$, the first term in the decomposition (3.5) is $\gamma_{0,1} t^\alpha$. Thus, apply Lemma 3.1 to $v(t) = t^\alpha$. Since the second term in the right-hand side of (3.8) vanishes when $\sigma = \alpha$, we get

$$|D_{RL}^\alpha v(t_m) - L_t^\alpha v(t_m)| \lesssim \tau^2 t_m^{-2} = m^{-2}.$$

Next, consider the other terms $\gamma_{j,k} t^{j+k\alpha}$ in (3.5). Applying Lemma 3.1 to $v(t) = t^\sigma$ with $\sigma \geq \gamma$, we get

$$\begin{aligned} |D_{RL}^\alpha v(t_m) - L_t^\alpha v(t_m)| &\lesssim \tau t_m^{\sigma-1-\alpha} + \tau^2 t_m^{\sigma-2-\alpha} \\ &= t_m^{\sigma-\gamma} t_m^{\gamma-\alpha} m^{-1} + t_m^{\sigma-\gamma} t_m^{\gamma-\alpha} m^{-2} \\ &\lesssim \tau^{\gamma-\alpha} m^{\gamma-\alpha-1}. \end{aligned}$$

Then the result follows. ☐

For the smooth term Y_2 in (3.5), which is not of the form t^σ, a different argument is necessary, which depends on the following special case of [15, Theorem 1].

Lemma 3.3. *Suppose that* $g \in C^1[0,T]$, $g'' \in L^1[0,T]$ *and* $g(0) = g'(0) = 0$. *Then*

$$|D_{RL}^\alpha g(t_m) - L_t^\alpha g(t_m)| \lesssim \tau \quad \textit{for } m = 1, 2, \ldots, M.$$

Lemma 3.4. *One has*

$$|D_{RL}^\alpha Y_2(t_m) - L_t^\alpha Y_2(t_m)| \lesssim \tau \quad \textit{for } m = 1, 2, \ldots, M.$$

Proof. This bound follows immediately from Lemma 3.3 (see also [16]), using the properties listed in (3.6). ☐

Now we can prove our global convergence result for the GL scheme.

Theorem 3.1. *Let* u *and* $\{U_m\}_{m=0}^M$ *be the solutions of* (3.1) *and* (3.7), *respectively. Then*

$$|u(t_m) - U_m| \lesssim \tau^\alpha \quad \textit{for } m = 1, \ldots, M.$$

Proof. Set $e_m = u(t_m) - U_m$ for $m = 0, \dots, M$. Subtraction of (3.7a) from (3.1a) gives

$$L_t^\alpha e_m + c(t_m)e_m = L_t^\alpha u(t_m) - D_{RL}^\alpha u(t_m) =: r_m. \tag{3.9}$$

Multiply this equation by e_m; then, using (2.5) and $d_k^{(\alpha)} - d_{k+1}^{(\alpha)} > 0$, it follows that

$$|e_m|^2 + c_m|e_m|^2 \le |r_m| \cdot |e_m| + \sum_{k=1}^{m} (d_k^{(\alpha)} - d_{k+1}^{(\alpha)})|e_{m-k}| \cdot |e_m|.$$

We can assume that $e_m \neq 0$ as otherwise the result is trivially true. Deleting the nonnegative term $c_m|e_m|^2$ from the inequality then dividing both sides by $|e_m|$, we get $L_t^\alpha|e_m| \le |r_m|$. But Lemmas 3.2 and 3.4 show that $|r_m| \lesssim m^{-2} + \tau^{\gamma-\alpha}m^{\gamma-\alpha-1} + \tau$, where $\gamma = \min\{1, 2\alpha\}$. From Lemma 2.2 it then follows that $|e_m| \lesssim \max_{j=1,\dots,m}\{t_j^\alpha |r_j|\} \lesssim \tau^\alpha$. □

4. Error analysis of the GL approximation away from $t = 0$

The analysis of Section 3 shows that the GL scheme yields $O(\tau^\alpha)$ accuracy when solving (3.1). But this is the worst-case error at all mesh points in $[0, T]$; in the present section we shall show that at all mesh points not close to $t = 0$, the GL scheme is more accurate — it is $O(\tau)$.

Imitating [17, (4.60)] and [6, (4.6)], define a sequence of stability multipliers $\{\sigma_n\}$ associated with the GL scheme by the recurrence relation

$$\sigma_0 := 1, \quad \sigma_n := \sum_{k=1}^{n} (d_k^{(\alpha)} - d_{k+1}^{(\alpha)})\sigma_{n-k} \ \text{ for } n = 1, 2, \dots \tag{4.1}$$

In [17, 6] analogous stability multipliers σ_n were used to analyse the L1 scheme, and in [7, (2.70)] and [18, (2.6)] the same idea was extended to a larger class of schemes. We shall use these multipliers in Theorem 4.1 to analyse the convergence away from $t = 0$ of the GL scheme (3.7) for (3.1), but unlike [17, 7, 18, 6] where the size of the multipliers can only be estimated for the L1 and other schemes, we shall derive an *exact explicit formula* for the σ_n of (4.1).

This exact formula is our next result. The key idea in its proof is the use of generating functions for the stability multipliers σ_n and for the coefficients $d_k^{(\alpha)}$.

Lemma 4.1. *The stability multipliers σ_n defined by* (4.1) *are given explicitly by*

$$\sigma_n = \frac{\Gamma(n+\alpha)}{\Gamma(\alpha)\Gamma(n+1)} \quad \textit{for } n = 0, 1, 2, \dots \tag{4.2}$$

Proof. By rearranging (4.1), one obtains

$$\sum_{k=1}^{n} d_k^{(\alpha)}\sigma_{n-k} = \sigma_n + \sum_{k=1}^{n} d_{k+1}^{(\alpha)}\sigma_{n-k} = \sum_{k=0}^{n} d_{k+1}^{(\alpha)}\sigma_{n-k} = \sum_{\ell=1}^{n+1} d_\ell^{(\alpha)}\sigma_{n+1-\ell}\,.$$

Hence $\sum_{k=1}^{n} d_k^{(\alpha)}\sigma_{n-k}$ is independent of n. To determine the value of this sum, take $n=1$; this gives

$$\sum_{k=1}^{n} d_k^{(\alpha)}\sigma_{n-k} = 1 \text{ for } n = 1, 2, \ldots. \tag{4.3}$$

Hence for $|x| < 1$ we get

$$\begin{aligned}
\frac{x}{1-x} &= \sum_{n=1}^{\infty} x^n = \sum_{n=1}^{\infty}\left(\sum_{k=1}^{n} d_k^{(\alpha)}\sigma_{n-k}\right)x^n \\
&= \sum_{k=1}^{\infty} d_k^{(\alpha)} x^k \left(\sum_{n=k}^{\infty}\sigma_{n-k}x^{n-k}\right) \\
&= x\left(\sum_{k=0}^{\infty} d_{k+1}^{(\alpha)}x^k\right)\left(\sum_{n=0}^{\infty}\sigma_n x^n\right),
\end{aligned}$$

where we used (4.3) then changed the order of summation. Now observe that the power series

$$\sum_{k=0}^{\infty} d_{k+1}^{(\alpha)}x^k = \sum_{k=0}^{\infty}\frac{\Gamma(k+1-\alpha)}{\Gamma(1-\alpha)\Gamma(k+1)}\,x^k = (1-x)^{\alpha-1} \quad \text{for } |x|<1;$$

the second equality is the binomial series expansion of $(1-x)^{\alpha-1}$ (see, e.g., [19, (5.13)]).

Substituting this identity into the previous equation yields

$$\sum_{n=0}^{\infty}\sigma_n x^n = (1-x)^{-\alpha} = \frac{1}{\Gamma(\alpha)}\sum_{n=0}^{\infty}\frac{\Gamma(n+\alpha)}{\Gamma(n+1)}\,x^n \quad \text{for } |x|<1,$$

where we again used a binomial series expansion. It follows that (4.2) is true. □

Remark 4.1. *Lemma 4.1 is valid in fact for all $\alpha > 0$.*

Corollary 4.1. *One has*

$$\frac{(n+1)^{\alpha-1}}{\Gamma(\alpha)} < \sigma_n < \frac{n^{\alpha-1}}{\Gamma(\alpha)} \quad \textit{for } n = 1, 2, \ldots \tag{4.4}$$

Proof. Use Gautschi's inequality [8] to estimate σ_n in (4.2). □

Our next result is a discrete stability bound analogous to [6, Lemma 4.2] for the L1 scheme; cf. [18, Theorem 3.2].

Lemma 4.2. *Let $\{U_m\}_{m=0}^{M}$ be the solution of (3.7). Then*

$$|U_m| \le \tau^\alpha \sum_{j=1}^{m}\sigma_{m-j}|f_j| \quad \textit{for} \quad m = 1, \ldots M. \tag{4.5}$$

Proof. We use induction on m to prove (4.5). The case $m = 1$ is immediate from (3.7) and (2.5). Suppose (4.5) is true for $m = 1, \dots, k-1$; we want to prove it for $m = k$.

As $U_0 = 0$, by using (2.5) one can rewrite (3.7a) (for $m = k$) as

$$\big[1 + c(t_k)\big]U_k = \tau^\alpha f_k + \sum_{l=1}^{k-1}(d_l^{(\alpha)} - d_{l+1}^{(\alpha)})U_{k-l}.$$

Now appeal to $c \geq 0, d_l^{(\alpha)} - d_{l+1}^{(\alpha)} > 0$ and the inductive hypothesis to get

$$\begin{aligned}
|U_k| &\leq \tau^\alpha |f_k| + \sum_{l=1}^{k-1}(d_l^{(\alpha)} - d_{l+1}^{(\alpha)})|U_{k-l}| \\
&\leq \tau^\alpha |f_k| + \sum_{l=1}^{k-1}(d_l^{(\alpha)} - d_{l+1}^{(\alpha)})\left[\tau^\alpha \sum_{j=1}^{k-l}\sigma_{k-l-j}|f_j|\right] \\
&= \tau^\alpha |f_k| + \tau^\alpha \sum_{j=1}^{k-1}|f_j| \sum_{l=1}^{k-j}(d_l^{(\alpha)} - d_{l+1}^{(\alpha)})\sigma_{k-l-j} \\
&= \tau^\alpha |f_k| + \tau^\alpha \sum_{j=1}^{k-1}|f_j|\sigma_{k-j} \\
&= \tau^\alpha \sum_{j=1}^{k}\sigma_{k-j}|f_j|,
\end{aligned}$$

where we used the definition (4.1). By the principle of induction, we are done. □

The following technical inequalities will be needed to finish our analysis.

Lemma 4.3. *Let $m \in \{1, 2, \dots, M\}$. Then*

$$\sum_{j=1}^{m} j^{-\beta}\sigma_{m-j} \lesssim \begin{cases} m^{\alpha-1} & \text{if } \beta > 1, \\ m^{\alpha-1}(\ln m + 1) & \text{if } \beta = 1, \\ m^{\alpha-\beta} & \text{if } 0 \leq \beta < 1. \end{cases}$$

Proof. Case $\beta > 1$: By (4.4) and $\sigma_0 = 1$, one has

$$\begin{aligned}
\sum_{j=1}^{m} j^{-\beta}\sigma_{m-j} &\leq m^{-\beta} + \frac{1}{\Gamma(\alpha)}\sum_{j=1}^{m-1} j^{-\beta}(m-j)^{\alpha-1} \\
&\lesssim m^{-\beta} + \left(\frac{m}{2}\right)^{\alpha-1}\sum_{j=1}^{\lceil m/2\rceil} j^{-\beta} + \left(\frac{m}{2}\right)^{\alpha-\beta}\sum_{j=\lceil m/2\rceil+1}^{m-1} j^{-\alpha}(m-j)^{\alpha-1} \\
&\lesssim m^{\alpha-1} + m^{\alpha-\beta}\int_{s=0}^{m} s^{-\alpha}(m-s)^{\alpha-1}\, ds \\
&\lesssim m^{\alpha-1},
\end{aligned}$$

where we used $\sum_1^n j^{-\beta} \lesssim 1$ and evaluated the Beta function integral by invoking [1, Theorem D.6].

Case $\beta = 1$: Repeating the argument for the case $\beta > 1$ leads to

$$\begin{aligned}\sum_{j=1}^{m} j^{-1}\sigma_{m-j} &\lesssim m^{-1} + \left(\frac{m}{2}\right)^{\alpha-1} \sum_{j=1}^{\lceil m/2 \rceil} j^{-1} + \left(\frac{m}{2}\right)^{\alpha-1} \sum_{j=\lceil m/2 \rceil+1}^{m-1} j^{-\alpha}(m-j)^{\alpha-1} \\ &\lesssim m^{\alpha-1}(\ln m + 1) + m^{\alpha-1} \int_{s=0}^{m} s^{-\alpha}(m-s)^{\alpha-1}\, ds \\ &\lesssim m^{\alpha-1}(\ln m + 1).\end{aligned}$$

Case $0 \le \beta < 1$: Again appealing to (4.4), $\sigma_0 = 1$, and [1, Theorem D.6] gives

$$\begin{aligned}\sum_{j=1}^{m} j^{-\beta}\sigma_{m-j} &\le m^{-\beta} + \frac{2^{1-\alpha}}{\Gamma(\alpha)} \sum_{j=1}^{m-1} \int_{s=j-1}^{j} s^{-\beta}(m-s)^{\alpha-1}\, ds \\ &\lesssim m^{-\beta} + \int_{s=0}^{m} s^{-\beta}(m-s)^{\alpha-1}\, ds \\ &\lesssim m^{-\beta} + m^{\alpha-\beta} \\ &\lesssim m^{\alpha-\beta}.\end{aligned}$$

□

We come now to the main result of the paper.

Theorem 4.1. *Let u and $\{U_m\}_{m=0}^M$ be the solutions of* (3.1) *and* (3.7)*, respectively. Then*

$$|u(t_m) - U_m| \lesssim \tau t_m^{\alpha-1} \quad \textit{for } m = 1, \dots, M.$$

Proof. Set $e_m = u(t_m) - U_m$ for $m = 0, \dots, M$. Subtracting (3.7a) from (3.1a), we get

$$L_t^\alpha e_m + c(t_m)e_m = L_t^\alpha u(t_m) - D_{RL}^\alpha u(t_m) =: r^m.$$

Hence, similarly to Lemma 4.2, one has $|e_m| \le \tau^\alpha \sum_{j=1}^m \sigma_{m-j}|r^j|$. But Lemmas 3.2 and 3.4 give us $|r_j| \lesssim j^{-2} + \tau^{\gamma-\alpha} j^{-(\alpha+1-\gamma)} + \tau$ with $\gamma = \min\{1, 2\alpha\}$, and now we can appeal to Lemma 4.3 to get

$$|e_m| \lesssim \tau^\alpha m^{\alpha-1} + \tau^\gamma m^{\gamma-1} + \tau^{1+\alpha} m^\alpha = \tau t_m^{\alpha-1} + \tau t_m^{\gamma-1} + \tau t_m^\alpha \lesssim \tau t_m^{\alpha-1}$$

using $t_m = m\tau$. □

Theorem 4.1 shows that "away from $t = 0$", i.e., for $t_m \ge \kappa > 0$ where κ is some fixed constant, the nodal error in the computed solution is $O(\tau)$. When the error is considered at all mesh points, Theorem 4.1 gives $O(\tau^\alpha)$ convergence, so it generalises the earlier result of Theorem 3.1. A similar phenomenon (improved order of convergence away from the initial time) has been observed in other settings; see for instance [17, Theorem 4] and [20, Theorem 3.4].

Remark 4.2. *Our proof of Theorem 4.1 is ultimately based on the generating function for the $d_k^{(\alpha)}$ that was employed in the proof of Lemma 4.1. Generating functions are also a fundamental tool in the analysis of [21], where convolution quadrature formulas for Riemann-Liouville integrals are investigated. In particular [21, Example 2.7] considers the generating function for the Grünwald-Letnikov coefficients $\omega_k^{(\alpha)}$, which were shown in Lemma 2.1 to have a close relationship to the $d_k^{(\alpha)}$, but the aim of [21] is the construction of methods that are accurate for all $t > 0$ (unlike the behaviour described in Theorem 4.1), so there is little overlap between that paper and ours.*

Remark 4.3. *In this paper we have considered only the 1-dimensional initial-value problem* (3.1)*, but there would be little difficulty in extending our results to initial-boundary value problems where the time derivative is $D^\alpha_{RL,t}u(x,t)$ and the initial condition is $u(\cdot, 0) = 0$. In [22], a numerical method for an initial-boundary value problem was analysed in this way; a pure initial-value problem was studied before proceeding to the analysis of the full space-time problem.*

5. Numerical results

We test the GL scheme (3.7) on an example of (3.1) whose solution is composed of the leading terms from (3.5).

Example 5.1. *Take $c = 2$ and $T = 1$ in* (3.1)*. Choose f such that $u(t) = t^\alpha + t^{2\alpha} + t^{1+\alpha}$ is the solution of* (3.1)*.*

Set $E1 := \max_{1\le m\le M} |U_m - u(t_m)|$ and $E2 := |U_M - u(t_M)|$, so $E1$ measures the global error and $E2$ measures the error at time $t = 1$. The numerical results in Tables 5.1 and 5.2 agree precisely with our theoretical bounds in Theorems 3.1 and 4.1. Note that the column $m = 0$ in [4, Table 4] — for a differential equation containing two fractional derivatives — also exhibits the $O(\tau)$ convergence away from $t = 0$ that is predicted by Theorem 4.1.

Table 5.1: Global errors and convergence rates

τ	$\alpha = 0.3$		$\alpha = 0.5$		$\alpha = 0.7$	
	$E1$	*Rate*	$E1$	*Rate*	$E1$	*Rate*
1/100	1.70e-02	0.20	8.14e-03	0.35	3.51e-03	0.91
1/200	1.49e-02	0.22	6.38e-03	0.40	1.86e-03	0.59
1/400	1.28e-02	0.23	4.84e-03	0.43	1.24e-03	0.64
1/800	1.09e-02	0.24	3.60e-03	0.45	7.96e-04	0.66
1/1600	9.23e-03	0.25	2.63e-03	0.47	5.03e-04	0.68
1/3200	7.76e-03		1.90e-03		3.14e-04	

Table 5.2: Errors and convergence rates at $t = 1$

τ	$\alpha = 0.3$		$\alpha = 0.5$		$\alpha = 0.7$	
	$E2$	$Rate$	$E2$	$Rate$	$E2$	$Rate$
1/100	6.44e-04	0.96	1.72e-03	0.99	3.51e-03	1.00
1/200	3.30e-04	0.97	8.66e-04	0.99	1.76e-03	1.00
1/400	1.68e-04	0.98	4.35e-04	1.00	8.80e-04	1.00
1/800	8.53e-05	0.98	2.18e-04	1.00	4.40e-04	1.00
1/1600	4.32e-05	0.99	1.09e-04	1.00	2.20e-04	1.00
1/3200	2.18e-05		5.47e-05		1.10e-04	

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